Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID: SSSPTA1626GMS

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

```
* * * * * *
                     Welcome to STN International
NEWS
                 Web Page URLs for STN Seminar Schedule - N. America
                 "Ask CAS" for self-help around the clock
NEWS
     2
NEWS 3
                 PATDPAFULL - New display fields provide for legal status
         FEB 28
                 data from INPADOC
         FEB 28
                BABS - Current-awareness alerts (SDIs) available
NEWS 4
NEWS 5
        MAR 02
                GBFULL: New full-text patent database on STN
NEWS
     6
        MAR 03
                 REGISTRY/ZREGISTRY - Sequence annotations enhanced
NEWS
     7
        MAR 03
                MEDLINE file segment of TOXCENTER reloaded
NEWS
        MAR 22
                KOREAPAT now updated monthly; patent information enhanced
                 Original IDE display format returns to REGISTRY/ZREGISTRY
NEWS
     9 MAR 22
NEWS 10 MAR 22
                 PATDPASPC - New patent database available
NEWS 11 MAR 22
                REGISTRY/ZREGISTRY enhanced with experimental property tags
NEWS 12 APR 04
                EPFULL enhanced with additional patent information and new
                 fields
NEWS 13 APR 04
                EMBASE - Database reloaded and enhanced
NEWS 14 APR 18
                New CAS Information Use Policies available online
NEWS 15 APR 25
                 Patent searching, including current-awareness alerts (SDIs),
                 based on application date in CA/CAplus and USPATFULL/USPAT2
                may be affected by a change in filing date for U.S.
                 applications.
NEWS
     16 APR 28
                 Improved searching of U.S. Patent Classifications for
                 U.S. patent records in CA/CAplus
     17 MAY 23
NEWS
                GBFULL enhanced with patent drawing images
NEWS
     18 MAY 23
                REGISTRY has been enhanced with source information from
                 CHEMCATS
NEWS
     19 JUN 06
                The Analysis Edition of STN Express with Discover!
                 (Version 8.0 for Windows) now available
NEWS
     20 JUN 13
                RUSSIAPAT: New full-text patent database on STN
NEWS
                FRFULL enhanced with patent drawing images
     21 JUN 13
NEWS 22 JUN 27
                MARPAT displays enhanced with expanded G-group definitions
                and text labels
NEWS 23 JUL 01
                MEDICONF removed from STN
NEWS
     24 JUL 07
                STN Patent Forums to be held in July 2005
NEWS 25 JUL 13
                SCISEARCH reloaded
NEWS 26 JUL 20
                Powerful new interactive analysis and visualization software,
                STN AnaVist, now available
                Derwent World Patents Index(R) web-based training during
NEWS
     27 AUG 11
                August
     28 AUG 11 STN AnaVist workshops to be held in North America
NEWS EXPRESS JUNE 13 CURRENT WINDOWS VERSION IS V8.0, CURRENT
             MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
```

AND CURRENT DISCOVER FILE IS DATED 13 JUNE 2005

NEWS HOURS STN Operating Hours Plus Help Desk Availability

NEWS INTER General Internet Information NEWS LOGIN Welcome Banner and News Items

NEWS PHONE Direct Dial and Telecommunication Network Access to STN

NEWS WWW CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

FILE 'HOME' ENTERED AT 08:36:59 ON 30 AUG 2005

=>

Uploading

THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE

Do you want to switch to the Registry File? Choice (Y/n):

Switching to the Registry File ...

Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> FILE REGISTRY

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 08:37:12 ON 30 AUG 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2005 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 29 AUG 2005 HIGHEST RN 862072-85-3 DICTIONARY FILE UPDATES: 29 AUG 2005 HIGHEST RN 862072-85-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

* The CR well and I have been a first to the control of the contro

* The CA roles and document type information have been removed from * the IDE default display format and the ED field has been added, *

10626155.trn

Structure search iteration limits have been increased. See HELP SLIMITS for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

Uploading C:\Program Files\Stnexp\Queries\10626155.str

chain nodes : 7 8 15 16 17 18 19 26 ring nodes : 1 2 3 4 5 6 9 10 11 12 13 14 20 21 22 23 chain bonds : 4-7 7-8 8-14 11-15 15-16 16-17 17-18 18-19 18-26 19-22 ring bonds : 1-2 1-6 2-3 3-4 4-5 5-6 9-10 9-14 10-11 11-12 12-13 13-14 20-21 20-25 21-22 22-23 23-24 24-25 exact/norm bonds : 11-15 15-16 17-18 18-19 exact bonds : 4-7 7-8 8-14 16-17 18-26 19-22 normalized bonds : 1-2 1-6 2-3 3-4 4-5 5-6 9-10 9-14 10-11 11-12 12-13 13-14 20-21 20-25 21-22 22-23 23-24 24-25 isolated ring systems : containing 1 : 9 : 20 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:CLASS

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

STR

Structure attributes must be viewed using STN Express query preparation.

SAMPLE SEARCH INITIATED 08:37:29 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 9 TO ITERATE

100.0% PROCESSED

9 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

9 TO 360

PROJECTED ANSWERS:

O TO

0 SEA SSS SAM L1

=> s l1 sss full

FULL SEARCH INITIATED 08:37:36 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 327 TO ITERATE

100.0% PROCESSED · 327 ITERATIONS

SEARCH TIME: 00.00.01

37 SEA SSS FUL L1

=> FIL HCAPLUS

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY

161.33

SESSION 161.54

37 ANSWERS

FULL ESTIMATED COST

10626155.trn Page 4

FILE 'HCAPLUS' ENTERED AT 08:37:44 ON 30 AUG 2005 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 30 Aug 2005 VOL 143 ISS 10 FILE LAST UPDATED: 29 Aug 2005 (20050829/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification. 1 hvertur

=> s 134 L3 L4

=> d l4 ibib abs hitstr tot

ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN 2005:78301 HCAPLUS

ACCESSION NUMBER:

DOCUMENT NUMBER: 142:176433

TITLE: A preparation of acetylenic compounds, useful in the

treatment of inflammatory disorders

Beers, Scott; Malloy, Elizabeth A.; Wachter, Michael INVENTOR(S):

PATENT ASSIGNEE(S): USĀ

SOURCE: U.S. Pat. Appl. Publ., 19 pp.

œ.

CODEN: USXXCO

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO. APPLICATION NO KIND DATE

US 2003-626155 US 2005020838 200503 **A**1 PRIORITY APPLN. INFO.: US 2003 626155

MARPAT 142:176433 OTHER SOURCE(S):

GΙ

appli salm

DATE

20030724

20030724

$$C1 - C \equiv C - C = 0$$
Me
Me
Me
III

AB The invention relates to a preparation of acetylenic compds. of formula I [wherein: A is cycloalkyldiyl, cyclic heteroalkyldiyl, or (hetero)aryldiyl; B is (hetero)aryldiyl; E is (hetero)aryldiyl; M and X are independently (CH2)0-4; R1 is cycloalkyl, cyclic heteroalkyl, or (hetero)aryl, etc.; R2 is H, alkyl, alkoxy, CHO, CO2H, or NH2, etc.; R3 and R4 are independently H, alkyl, CHO, cycloalkyl, or aryl, etc.], useful in the treatment of inflammatory disorders. For instance, acetylene derivative II (oxidase inhibition: IC50 = 0.7 μM) was prepared via reductive amination of ketone III by 1,4-bis(aminomethyl)benzene.

651330-36-8P 651330-37-9P 651330-38-0P 651330-39-1P 651330-44-8P 651330-45-9P 651330-46-0P 651330-47-1P 651330-48-2P 651330-49-3P 651330-50-6P 651330-51-7P 651330-52-8P 651330-53-9P 651330-54-0P 651330-55-1P 651330-58-4P 651330-59-5P 651330-61-9P 651330-63-1P 651330-64-2P 651330-65-3P 651330-68-6P 773847-69-1P 776293-45-9P 792905-81-8P 832116-38-8P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of acetylenic compound useful in the treatment of inflammatory disorders)

RN 651330-36-8 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[4-[(4-chlorophenyl)ethynyl]-2-methylphenoxy]-1-methylethyl]- (9CI) (CA INDEX NAME)

10626155.trn

Page 6

RN 651330-37-9 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[4-[(4-chlorophenyl)ethynyl]-2-methylphenoxy]-1-methylethyl]-, dihydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{C1} \\ \text{C2} \\ \text{C2} \\ \text{C3} \\ \text{C4} \\ \text{C1} \\ \text{C2} \\ \text{C4} \\ \text{C2} \\ \text{C2} \\ \text{C4} \\ \text{C2} \\ \text{C4} \\ \text{C5} \\ \text{C6} \\ \text{C7} \\ \text{C6} \\ \text{C7} \\ \text{C7} \\ \text{C7} \\ \text{C8} \\$$

●2 HC1

RN 651330-38-0 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[2-chloro-4-(phenylethynyl)phenoxy]-1methylethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{CH}_2\text{NH-CH-CH}_2\text{-O} \\ \text{Cl} \end{array}$$

RN 651330-39-1 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[1-[[4-[(4-chlorophenyl)ethynyl]-2-methylphenoxy]methyl]propyl]- (9CI) (CA INDEX NAME)

RN 651330-44-8 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[4-[(4-chlorophenyl)ethynyl]phenoxy]ethyl]-N'-propyl- (9CI) (CA INDEX NAME)

RN 651330-45-9 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[4-[(4-chlorophenyl)ethynyl]-2-methylphenoxy]ethyl]-N'-propyl- (9CI) (CA INDEX NAME)

RN 651330-46-0 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[4-[(4-chlorophenyl)ethynyl]phenoxy]ethyl]-N'-(1-methylethyl)- (9CI) (CA INDEX NAME)

RN 651330-47-1 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[4-[(4-chlorophenyl)ethynyl]phenoxy]ethyl]-N'-(3-methylbutyl)- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

RN 651330-48-2 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[4-[(4-chlorophenyl)ethynyl]-2-methylphenoxy]ethyl]-N'-(3-methylbutyl)- (9CI) (CA INDEX NAME)

PAGE 1-B

RN 651330-49-3 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[4-[(4-chlorophenyl)ethynyl]phenoxy]ethyl]-N'-[3-(dimethylamino)propyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

$$Me_2N-(CH_2)_3-NH-CH_2$$
 $CH_2-NH-CH_2-CH_2-O$

PAGE 1-B

RN 651330-50-6 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[4-[(4-chlorophenyl)ethynyl]-2-methylphenoxy]ethyl]-N'-(phenylmethyl)- (9CI) (CA INDEX NAME)

PAGE 1-A

$$\begin{array}{c} \text{Ph-CH}_2-\text{NH-CH}_2 \\ \hline \\ \text{CH}_2-\text{NH-CH}_2-\text{CH}_2-\text{O} \\ \hline \end{array}$$

PAGE 1-B

RN 651330-51-7 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[4-[(4-chlorophenyl)ethynyl]-2-methylphenoxy]ethyl]-N'-heptyl- (9CI) (CA INDEX NAME)

PAGE 1-A

Me—
$$(CH_2)_6$$
— NH — CH_2 — CH_2 — NH — CH_2 —

PAGE 1-B

RN 651330-52-8 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[4-[(4-chlorophenyl)ethynyl]-2-methylphenoxy]ethyl]-N'-(3-phenylpropyl)- (9CI) (CA INDEX NAME)

PAGE 1-A

$$Ph-(CH_2)_3-NH-CH_2$$
 Me $CH_2-NH-CH_2-CH_2-O$

PAGE 1-B

RN 651330-53-9 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[4-[(4-chlorophenyl)ethynyl]-2-methylphenoxy]ethyl]-N'-decyl- (9CI) (CA INDEX NAME)

$$Me^{-(CH_2)} = NH - CH_2$$
 $CH_2 - NH - CH_2 - CH_2 - O$
 Me
 $CH_2 - NH - CH_2 - CH_2 - O$

08/30/2005

10626155.trn

PAGE 1-B

RN 651330-54-0 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[4-[(4-chlorophenyl)ethynyl]-2-methylphenoxy]ethyl]-N'-hexyl- (9CI) (CA INDEX NAME)

PAGE 1-A

$$Me^{-(CH_2)} = NH - CH_2$$

$$CH_2 - NH - CH_2 - CH_2 - O$$

$$Me$$

PAGE 1-B

RN 651330-55-1 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[4-[(4-chlorophenyl)ethynyl]-2-methylphenoxy]ethyl]-N'-[2-(1-methyl-2-pyrrolidinyl)ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-B

RN 651330-58-4 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[4-[(4-chlorophenyl)ethynyl]-2-methylphenoxy]ethyl]-N'-[2-(1-pyrrolidinyl)ethyl]- (9CI) (CA INDEX NAME)

08/30/2005

10626155.trn

PAGE 2-A

RN 651330-59-5 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[4-[(4-chlorophenyl)ethynyl]-2-methylphenoxy]ethyl]-N'-[3-(4-morpholinyl)propyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

$$-(CH2)3-N$$

RN 651330-61-9 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[4-[(4-chlorophenyl)ethynyl]-2-methylphenoxy]ethyl]-N'-[2-(4-morpholinyl)ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

RN 651330-63-1 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[4-[(4-chlorophenyl)ethynyl]-2-methylphenoxy]ethyl]-N'-phenyl- (9CI) (CA INDEX NAME)

RN 651330-64-2 HCAPLUS

CN 2-Piperidinecarboxylic acid, 3-[[[4-[[[2-[4-[(4-chlorophenyl)ethynyl]-2-methylphenoxy]ethyl]amino]methyl]phenyl]methyl]amino]propyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

$$C = C + CH_2 - CH_2 - NH - CH_2 - NH$$

PAGE 1-B

$$-(CH2)3-0-C$$

10626155.trn

Page 14

08/30/2005

10626155.trn

RN 651330-65-3 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[4-[(4-chlorophenyl)ethynyl]-2-methylphenoxy]ethyl]-N'-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

RN 651330-68-6 HCAPLUS

CN: 1,4-Benzenedimethanamine, N-[2-[4-[(4-chlorophenyl)ethynyl]-2-methylphenoxy]ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{CH}_2\text{N-CH}_2 \\ \text{CH}_2\text{-NH-CH}_2\text{-CH}_2\text{-O} \end{array}$$

RN 773847-69-1 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[2-chloro-4-[(4-fluorophenyl)ethynyl]phenoxy]-1-methylethyl]- (9CI) (CA INDEX NAME)

RN 776293-45-9 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[2-chloro-4-[(4-chlorophenyl)ethynyl]phenoxy]-1-methylethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{C1} & \text{Me} \\ \hline \\ \text{C1} & \text{CH}_2-\text{NH}_2 \\ \hline \\ \text{C} & \text{CH}_2-\text{NH}_2 \\ \hline \end{array}$$

RN .792905-81-8 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[2-chloro-4-[(4-methylphenyl)ethynyl]phenoxy]-1-methylethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{O-CH}_2\text{-CH-NH-CH}_2 \end{array}$$

RN 832116-38-8 HCAPLUS

CN 1,4-Benzenedimethanamine, N-butyl-N'-[2-[4-[(4-chlorophenyl)ethynyl]-2methylphenoxy]ethyl]-N-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{n-Bu-N-CH}_2 \\ \text{CH}_2\text{-NH-CH}_2\text{-CH}_2\text{-O} \end{array}$$

IT 651330-74-4P

> RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of acetylenic compound useful in the treatment of inflammatory disorders)

RN 651330-74-4 HCAPLUS

CNBenzaldehyde, 4-[[[2-[4-[(4-chlorophenyl)ethynyl]phenoxy]ethyl]amino]methy 1] - (9CI) (CA INDEX NAME)

ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

2004:650899 HCAPLUS

DOCUMENT NUMBER:

141:173978

TITLE:

Preparation of aminoacetonitrile derivatives as

agricultural and horticultural insecticides

INVENTOR (S):

Andoh, Nobuharu; Sanpei, Osamu; Sakata, Kazuyuki Nihon Nohyaku Co., Ltd., Japan

PATENT ASSIGNEE(S): SOURCE:

Eur. Pat. Appl., 48 pp.

CODEN: EPXXDW

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND DATE	APPLICATION NO.	DATE
EP 1445251	A1 20040811	EP 2004-10346	19990428
R: CH, DĒ, FR, EP 953565	GB, CT, LI A2 19991103	EP 1999-107461	19990428
EP 953565	A3 20021204		

10626155.trn

Page 16

EP 953565 B1 20040908

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO

PRIORITY APPLN. INFO.:

JP 1998-137806

A 19980501

OTHER SOURCE(S):

EP 1999-107461

A3 19990428

1 mules

MARPAT 141:173978

GT

AB The title compds. Ar1(Q)dC(O)NR3C(CN)R4(CR5R6)aW(CR7R8)bAr2 [I; Ar1, Ar2 = (substituted) Ph, (substituted) phenyloxy, (substituted) phenylacetylene; (substituted) pyridyl and (substituted) naphthyl; Q = CR1R2 (wherein R1, R2 = H, halo, (halo)alkyl, etc.); R3 = H, (halo)alkyl, etc.; R4-R8 = H, halo, (halo)alkyl, etc.; W = O, S, SO2 or NR9 (wherein R9 = H, alkyl); a, b = 0-4; d = 0-1], useful as insecticides, were prepared E.g., a multi-step synthesis of II (starting from 4-chlorophenol and bromoacetaldehyde dimethylacetal), was given. The compds. I were tested against diamondback moth and against smaller tea tortrix (data were given for representative compds. I).

ΙT 736172-93-3P

> RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of aminoacetonitrile derivs, as agricultural and horticultural insecticides)

RN736172-93-3 HCAPLUS

Benzamide, 4-chloro-N-[1-cyano-1-methyl-2-[4-(phenylethynyl)phenoxy]ethyl]-CN(9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Ph-C} \\ \text{C} \\ \text{O-CH}_2 \\ \text{CN} \end{array} \begin{array}{c} \text{Me} \\ \text{O} \\ \text{CN} \end{array} \begin{array}{c} \text{Cl} \\ \text$$

ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

2004:80636 HCAPLUS

DOCUMENT NUMBER:

140:145889

TITLE:

Dreparation of acetylenic-aryl-methylamines useful in

treating inflammatory disorders

Beers, Scott; Marloy, Elizabeth A.; Wachter, Michael

PATENT ASSIGNEE(S)

Janssen Pharmaceutica N.V., Belg. PCT Int. Appl., 61 pp.

SOURCE:

CODEN: PIXXD2

DOCUMENT TYPE:

INVENTOR(S):

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

10626155.trn

Page 17

PATENT INFORMATION:

```
PATENT NO.
                         KIND
                                 DATE
                                            APPLICATION NO.
                                                                     DATE
     -----
                         ----
                                 -----
                                             -----
     WO 2004009531
                          A1
                                 20040129
                                            WO 2003-US23140
                                                                     20030724
        W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,
             PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN,
             TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
             FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
                                             US 2002-398138P P 20020724
PRIORITY APPLN. INFO.:
OTHER SOURCE(S):
                         MARPAT 140:145889
```

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [A = cycloalkyldiyl, cyclic heteroalkyldiyl, etc.; B, E = (hetero)aryldiyl; Rl = cycloalkyl, cyclic heteroalkyl, heteroaryl, etc.; R2 = H, alkanyl, alkoxy, acyl, etc.; R3-4 = H, alkanyl, carboxy, cycloalkyl, etc.] are prepared For instance, 4-iodo-2-methylphenol is alkylated with chloroacetone (acetone, K2CO3, NaI, reflux, 18 h), the product coupled to 4-chlorophenylacetylene (Pd(II), Et3N) and used to alkylate p-xylylene diamine (CH2Cl2, HOAc, NaBH(OAc)3) to give II. In an NADPH oxidase assay for inhibition of superoxide-mediated reduction of cytochrome C in human neutrophils incubated with phorbol myristate acetate, 26 compds. I had IC50 values of 0.7-11.13 μ M; II had IC50 = 0.7 μ M. I are useful in treating or ameliorating reactive oxygen species-mediated inflammatory disorders.

```
Species-mediated inflammatory disorders.

IT 651330-36-8P 651330-37-9P 651330-38-0P
651330-39-1P 651330-40-4P 651330-41-5P
651330-42-6P 651330-43-7P 651330-44-8P
651330-45-9P 651330-46-0P 651330-50-6P
651330-51-7P 651330-52-8P 651330-53-9P
651330-54-0P 651330-55-1P 651330-57-3P
651330-68-4P 651330-59-5P 651330-61-9P
651330-66-4P 651330-68-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
```

(Uses)
 (preparation of acetylenic-aryl-methylamines as NAD oxidase hydride donor
 inhibitors useful in treating reactive oxygen species-mediated

inflammatory disorders)
RN 651330-36-8 HCAPLUS

1,4-Benzenedimethanamine, N-[2-[4-[(4-chlorophenyl)ethynyl]-2methylphenoxy]-1-methylethyl]- (9CI) (CA INDEX NAME) 08/30/2005

10626155.trn

$$\begin{array}{c} \text{Me} \\ \text{O-CH}_2\text{-CH-NH-CH}_2 \end{array}$$

RN 651330-37-9 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[4-[(4-chlorophenyl)ethynyl]-2-methylphenoxy]-1-methylethyl]-, dihydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{C1} \\ \text{C2} \\ \text{C2} \\ \text{C3} \\ \text{C4} \\ \text{C5} \\ \text{C6} \\ \text{C6} \\ \text{C7} \\ \text{C6} \\ \text{C7} \\ \text{C6} \\ \text{C7} \\ \text{C7} \\ \text{C7} \\ \text{C8} \\$$

●2 HCl

RN 651330-38-0 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[2-chloro-4-(phenylethynyl)phenoxy]-1-methylethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{CH}_2\text{NH-CH-CH}_2\text{-O} \\ \text{Cl} \end{array}$$

RN 651330-39-1 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[1-[[4-[(4-chlorophenyl)ethynyl]-2-methylphenoxy]methyl]propyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{C1} & \text{Et} & \text{CH}_2-\text{NH}_2 \\ \hline \\ \text{C} & \text{C} & \text{CH}_2-\text{CH}-\text{NH}-\text{CH}_2 \\ \hline \end{array}$$

RN 651330-40-4 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[1-[[4-[(4-chlorophenyl)ethynyl]-2-methylphenoxy]methyl]propyl]-, dihydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{C1} \\ \text{C1} \\ \text{C2} \\ \text{C2} \\ \text{C3} \\ \text{C4} \\ \text{C5} \\ \text{C6} \\ \text{C6} \\ \text{C7} \\ \text{C6} \\ \text{C7} \\ \text{C7} \\ \text{C8} \\$$

●2 HCl

RN 651330-41-5 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[2-chloro-4-[(4-methylphenyl)ethynyl]phenoxy]-1-methylethyl]-, dihydrochloride (9CI) (CP INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \text{CH}_2-\text{NH}_2 \\ \hline \\ \text{O-CH}_2-\text{CH-NH-CH}_2 \\ \hline \end{array}$$

● 2 HCl

RN 651330-42-6 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[2-chloro-4-[(4-chlorophenyl)ethynyl]phenoxy]-1-methylethyl]-, dihydrochloride (9CI) (CAINDEX NAME)

●2 HCl

RN 651330-43-7 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[2-chloro-4-[(4-fluorophenyl)ethynyl]phenoxy]-1-methylethyl]-, dihydrochloride (9CI) (CAINDEX NAME)

•2 HCl

RN 651330-44-8 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[4-[(4-chlorophenyl)ethynyl]phenoxy]ethyl]-N'-propyl- (9CI) (CA INDEX NAME)

RN 651330-45-9 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[4-[(4-chlorophenyl)ethynyl]-2-methylphenoxy]ethyl]-N'-propyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{N-PrNH-CH}_2 \\ \text{CH}_2 - \text{NH-CH}_2 - \text{CH}_2 - \text{O} \end{array}$$

RN 651330-46-0 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[4-[(4-chlorophenyl)ethynyl]phenoxy]ethyl]-N'-(1-methylethyl)- (9CI) (CA INDEX NAME)

RN 651330-47-1 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[4-[(4-chlorophenyl)ethynyl]phenoxy]ethyl]-N'-(3-methylbutyl)- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

RN 651330-48-2 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[4-[(4-chlorophenyl)ethynyl]-2-methylphenoxy]ethyl]-N'-(3-methylbutyl)- (9CI) (CA INDEX NAME)

PAGE 1-A

$$\label{eq:ch_ch_2} \text{Me}_2\text{CH}-\text{CH}_2-\text{CH}_2-\text{NH}-\text{CH}_2\\ \text{CH}_2-\text{NH}-\text{CH}_2-\text{CH}_2-\text{O}\\ \text{CH}_2-\text{CH}_2-\text{CH}_2-\text{O}\\ \text{CH}_2-\text{CH}_2$$

PAGE 1-B

RN 651330-49-3 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[4-[(4-chlorophenyl)ethynyl]phenoxy]ethyl]-N'-[3-(dimethylamino)propyl]- (9CI) (CA INDEX NAME)

$$Me_2N-(CH_2)_3-NH-CH_2$$
 $CH_2-NH-CH_2-CH_2-O$

PAGE 1-B

Cl

RN 651330-50-6 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[4-[(4-chlorophenyl)ethynyl]-2-methylphenoxy]ethyl]-N'-(phenylmethyl)- (9CI) (CA INDEX NAME)

PAGE 1-A

$$\begin{array}{c} \text{Ph-CH}_2-\text{NH-CH}_2 \\ \hline \\ \text{CH}_2-\text{NH-CH}_2-\text{CH}_2-\text{O} \\ \hline \end{array}$$

PAGE 1-B

RN 651330-51-7 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[4-[(4-chlorophenyl)ethynyl]-2-methylphenoxy]ethyl]-N'-heptyl- (9CI) (CA INDEX NAME)

PAGE .1-A

Me—
$$(CH_2)_6$$
— NH — CH_2 — CH_2 — NH — CH_2 —

PAGE 1-B

RN 651330-52-8 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[4-[(4-chlorophenyl)ethynyl]-2-methylphenoxy]ethyl]-N'-(3-phenylpropyl)- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

RN 651330-53-9 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[4-[(4-chlorophenyl)ethynyl]-2-methylphenoxy]ethyl]-N'-decyl- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

RN 651330-54-0 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[4-[(4-chlorophenyl)ethynyl]-2-methylphenoxy]ethyl]-N'-hexyl- (9CI) (CA INDEX NAME)

PAGE 1-B

RN 651330-55-1 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[4-[(4-chlorophenyl)ethynyl]-2-methylphenoxy]ethyl]-N'-[2-(1-methyl-2-pyrrolidinyl)ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

RN 651330-57-3 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[4-[(4-chlorophenyl)ethynyl]-2-methylphenoxy]ethyl]-N'-[2-(1-methyl-2-pyrrolidinyl)ethyl]-, trihydrochloride (9CI) (CA INDEX NAME)

PAGE 1-A

$$\begin{array}{c} \text{Me} \\ \\ \text{N} \\ \text{CH}_2\text{-}\text{CH}_2\text{-}\text{NH}\text{-}\text{CH}_2\\ \\ \text{CH}_2\text{-}\text{NH}\text{-}\text{CH}_2\text{-}\text{CH}_2\text{-}\text{O} \end{array}$$

●3 HC1

PAGE 1-B

RN 651330-58-4 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[4-[(4-chlorophenyl)ethynyl]-2-methylphenoxy]ethyl]-N'-[2-(1-pyrrolidinyl)ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

- RN 651330-59-5 HCAPLUS
- CN 1,4-Benzenedimethanamine, N-[2-[4-[(4-chlorophenyl)ethynyl]-2-methylphenoxy]ethyl]-N'-[3-(4-morpholinyl)propyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

RN 651330-61-9 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[4-[(4-chlorophenyl)ethynyl]-2-methylphenoxy]ethyl]-N'-[2-(4-morpholinyl)ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

RN 651330-63-1 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[4-[(4-chlorophenyl)ethynyl]-2-methylphenoxy]ethyl]-N'-phenyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{PhNH-CH}_2 \\ \text{CH}_2 - \text{NH-CH}_2 - \text{CH}_2 - \text{O} \end{array}$$

RN 651330-64-2 HCAPLUS

CN 2-Piperidinecarboxylic acid, 3-[[[4-[[[2-[4-[(4-chlorophenyl)ethynyl]-2-methylphenoxy]ethyl]amino]methyl]phenyl]methyl]amino]propyl ester (9CI)

10626155.trn

Page 28

(CA INDEX NAME)

PAGE 1-A

$$\begin{array}{c} \text{Me} \\ \text{O-CH}_2\text{-CH}_2\text{-NH-CH}_2 \\ \text{CH}_2\text{-NH-} \end{array}$$

PAGE 1-B

RN 651330-65-3 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[4-[(4-chlorophenyl)ethynyl]-2-methylphenoxy]ethyl]-N'-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

RN 651330-66-4 HCAPLUS

CN 1,4-Benzenedimethanamine, N-butyl-N'-[2-[4-[(4-chlorophenyl)ethynyl]-2-methylphenoxy]ethyl]- (9CI) (CA INDEX NAME)

RN 651330-68-6 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[4-[(4-chlorophenyl)ethynyl]-2-methylphenoxy]ethyl]- (9CI) (CA INDEX NAME)

IT 651330-73-3P 651330-74-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of acetylenic-aryl-methylamines as NAD oxidase hydride donor inhibitors useful in treating reactive oxygen species-mediated inflammatory disorders)

RN 651330-73-3 HCAPLUS

CN Benzenemethanamine, N-[2-[4-[(4-chlorophenyl)ethynyl]phenoxy]ethyl]-4-(diethoxymethyl)- (9CI) (CA INDEX NAME)

RN 651330-74-4 HCAPLUS

CN Benzaldehyde, 4-[[[2-[4-[(4-chlorophenyl)ethynyl]phenoxy]ethyl]amino]methy 1]- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN

5

ACCESSION NUMBER:

1999:708444 HCAPLUS

DOCUMENT NUMBER:

131:310455

TITLE:

Preparation of aroylaminoacetonitriles as agricultural

and horticultural insecticides

INVENTOR(S):
PATENT ASSIGNEE(S):

Andoh, Nobuharu; Sanpei, Osamu; Sakata, Kazuyuki

Nihon Nohyaku Co., Ltd., Japan

SOURCE:

Eur. Pat. Appl., 63 pp.

CODEN: EPXXDW

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 953565	A2	19991103 .	EP 1999-107461	19990428

10626155.trn

Page 30

					A3 B1													
	R:	AT,	BE,	CH,	DE,	DK, I	ES,	FR,	GB,	GF	≀, I	Т,	LI,	LU,	NL,	SE	, MC	, PT
													•	•	•		•	
US	62390)77	>		B1	2.0	0010	529		US	199	9-2	953	19			1999	0421
TW	58584	19			В	20	040	501		TW	199	9-8	810	6732			1999	0427
EΡ	14452	251			A1	20	040	811		ΕP	200	4 - 1	034	6			1999	0428
	R:	CH,	DE,	FR,	GB,	IT, I	LΙ											
CN	12341	L77			Α	19	9991	.110		CN	199	9-1	052	89			19990	0430
CN	11325	516			В	20	0031	231										
ΑU	99260)27			A1	19	9991	111		AU	199	9-2	602	7			19990	0430
ΑU	75211	L2			B2	20	020	905										
JP	20000	2639	92		A2	20	0000	125		JP	199	9-1	245	60			19990	0430
ORITY	APPI	LN.]	INFO	. :						JP	199	8-1	.378	06	1	Ą	1998	0501
										EΡ	199	9-1	074	61	1	43	19990	0428
	EP US TW EP CN CN AU AU JP	EP 95356 R: US 62390 TW 58584 EP 14452 R: CN 12342 CN 11325 AU 99260 AU 75211 JP 20000	IE, US 6239077 TW 585849 EP 1445251 R: CH, CN 1234177 CN 1132516 AU 9926027 AU 752112 JP 200002639	EP 953565 R: AT, BE, IE, SI, US 6239077 TW 585849 EP 1445251 R: CH, DE, CN 1234177 CN 1132516 AU 9926027 AU 752112 JP 2000026392	EP 953565 R: AT, BE, CH, IE, SI, LT, US 6239077 FW 585849 EP 1445251 R: CH, DE, FR, CN 1234177 CN 1132516 AU 9926027 AU 752112	EP 953565 B1 R: AT, BE, CH, DE, IE, SI, LT, LV, US 6239077 B1 TW 585849 B EP 1445251 A1 R: CH, DE, FR, GB, CN 1234177 A CN 1132516 B AU 9926027 A1 AU 752112 B2 JP 2000026392 A2	EP 953565 B1 20 R: AT, BE, CH, DE, DK, I IE, SI, LT, LV, FI, I US 6239077 B1 20 FW 585849 B 20 EP 1445251 A1 20 R: CH, DE, FR, GB, IT, I CN 1234177 A 19 CN 1132516 B 20 AU 9926027 A1 19 AU 752112 B2 20 JP 2000026392 A2 20	EP 953565 B1 20040 R: AT, BE, CH, DE, DK, ES,	EP 953565 R: AT, BE, CH, DE, DK, ES, FR, IE, SI, LT, LV, FI, RO US 6239077 B1 20010529 TW 585849 EP 1445251 R: CH, DE, FR, GB, IT, LI CN 1234177 CN 1132516 B 20031231 AU 9926027 A1 19991111 AU 752112 B2 20020905 JP 2000026392 A2 20000125	EP 953565 B1 20040908 R: AT, BE, CH, DE, DK, ES, FR, GB, IE, SI, LT, LV, FI, RO US 6239077 B1 20010529 TW 585849 B 20040501 EP 1445251 A1 20040811 R: CH, DE, FR, GB, IT, LI CN 1234177 A 19991110 CN 1132516 B 20031231 AU 9926027 A1 19991111 AU 752112 B2 20020905 JP 2000026392 A2 20000125 ORITY APPLN. INFO.:	EP 953565 R: AT, BE, CH, DE, DK, ES, FR, GB, GF IE, SI, LT, LV, FI, RO US 6239077 B1 20010529 US 6239077 B1 20040501 TW 585849 EP 1445251 R: CH, DE, FR, GB, IT, LI CN 1234177 CN 1132516 B 20031231 AU 9926027 A1 19991111 AU 752112 B2 20020905 JP 2000026392 ORITY APPLN. INFO.:	EP 953565 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, I IE, SI, LT, LV, FI, RO US 6239077 B1 20010529 US 199 EP 1445251 R: CH, DE, FR, GB, IT, LI CN 1234177 CN 1132516 AU 9926027 AU 752112 B2 20020905 JP 2000026392 ORITY APPLN. INFO.: UK, ES, FR, GB, GR, I II	EP 953565 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, IE, SI, LT, LV, FI, RO US 6239077 B1 20010529 EV 1445251 R: CH, DE, FR, GB, IT, LI CN 1234177 CN 1132516 A1 19991110 CN 1999-1 CN 19926027 A1 19991111 AU 1999-2 AU 752112 B2 20020905 JP 2000026392 A2 20000125 JP 1998-1	EP 953565 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, IE, SI, LT, LV, FI, RO US 6239077 B1 20010529 US 1999-2953 TW 585849 B 20040501 TW 1999-8810 EP 1445251 A1 20040811 EP 2004-1034 R: CH, DE, FR, GB, IT, LI CN 1234177 A 19991110 CN 1999-1052 CN 1132516 B 20031231 AU 9926027 A1 19991111 AU 1999-2602 AU 752112 B2 20020905 JP 2000026392 A2 20000125 JP 1998-1378	EP 953565 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, IE, SI, LT, LV, FI, RO US 6239077 B1 20010529 US 1999-295319 EV 585849 B 20040501 TW 1999-88106732 EP 1445251 A1 20040811 EP 2004-10346 R: CH, DE, FR, GB, IT, LI CN 1234177 A 19991110 CN 1999-105289 CN 1132516 B 20031231 AU 9926027 AU 752112 B2 20020905 JP 1999-124560	EP 953565 B1 20040908 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, IE, SI, LT, LV, FI, RO US 6239077 B1 20010529 US 1999-295319 TW 585849 B 20040501 TW 1999-88106732 EP 1445251 A1 20040811 EP 2004-10346 R: CH, DE, FR, GB, IT, LI CN 1234177 A 19991110 CN 1999-105289 CN 1132516 B 20031231 AU 9926027 A1 19991111 AU 1999-26027 AU 752112 B2 20020905 JP 2000026392 A2 20000125 JP 1999-124560 ORITY APPLN. INFO.: JP 1998-137806	EP 953565 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE IE, SI, LT, LV, FI, RO US 6239077 B1 20010529 US 1999-295319 TW 585849 B 20040501 TW 1999-88106732 EP 1445251 A1 20040811 EP 2004-10346 R: CH, DE, FR, GB, IT, LI CN 1234177 A 19991110 CN 1999-105289 CN 1132516 B 20031231 AU 9926027 AI 19991111 AU 1999-26027 AU 752112 B2 20020905 JP 2000026392 A2 20000125 JP 1999-124560 ORITY APPLN. INFO.: JP 1998-137806 A	EP 953565 B1 20040908 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC IE, SI, LT, LV, FI, RO US 6239077 B1 20010529 US 1999-295319 19990 TW 585849 B 20040501 TW 1999-88106732 19990 EP 1445251 A1 20040811 EP 2004-10346 19990 R: CH, DE, FR, GB, IT, LI CN 1234177 A 19991110 CN 1999-105289 19990 CN 1132516 B 20031231 AU 9926027 A1 19991111 AU 1999-26027 19990 AU 752112 B2 20020905 JP 2000026392 A2 20000125 JP 1999-124560 19990 ORITY APPLN. INFO.: JP 1998-137806 A 19980

OTHER SOURCE(S): MARPAT 131:310455

APIQCONR3C(CN)R4(CR5R6)aW(CR7R8)bAr2 [I; Ar1, Ar2 = (substituted) Ph, PhO, pyridyl, pyridyloxy, naphthyl; Q = CR1R2; R1, R2 = H, halo, (halo)alkyl, (halo)alkoxy, (substituted) cycloalkyl; R1R2 = (substituted) C2-6 alkylene, CH:CH, C.tplbond.C; d = 0, 1; R3 = H, (halo)alkyl; R4-R8 = H, halo, (halo)alkyl; W = O, S, SO2, NR9; R9 = H, alkyl; a, b = 0-4], were prepared Thus, 4-chlorophenol, bromoacetaldehyde di-Me acetal, K2CO3, and cat. NaI were refluxed 3 h in DMF to give 4-chlorophenoxyacetaldehyde di-Me acetal. This was refluxed with aqueous HCl in acetone to give crude 4-chlorophenoxyacetaldehyde, which was stirred with NaCN and NH4Cl in aqueous NH3 to give a reside. This was stirred with 4-chlorophenylacetyl chloride and Et3N in THF to give I (Ar1, Ar2 = 4-ClC6H4; R1-R8 = H; W = O; a, d = 1; b = 0). Numerous I at 500 ppm gave 100% kill of Plutella xylostella on cabbage seedlings.

IT 247199-30-0P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of aroylaminoacetonitriles as agricultural and horticultural insecticides)

RN 247199-30-0 HCAPLUS

CN Benzamide, N-[1-cyano-1-methyl-2-[4-(phenylethynyl)phenoxy]ethyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

=> FIL REGISTRY COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 44.26 205.80 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION CA SUBSCRIBER PRICE -2.92 -2.92

FILE 'REGISTRY' ENTERED AT 08:43:44 ON 30 AUG 2005

10626155.trn

Page 31

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2005 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 29 AUG 2005 HIGHEST RN 862072-85-3 DICTIONARY FILE UPDATES: 29 AUG 2005 HIGHEST RN 862072-85-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Structure search iteration limits have been increased. See HELP SLIMITS for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

Uploading C:\Program Files\Stnexp\Queries\10626155a.str

chain nodes :

7 8 15 16 17 18 19 26 28 29

ring nodes :

1 2 3 4 5 6 9 10 11 12 13 14 20 21 22 23 24 25 chain bonds:

10626155.trn

Page 32

4-7 7-8 8-14 11-15 15-16 16-17 17-18 18-19 18-26 19-22 28-29

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 9-10 9-14 10-11 11-12 12-13 13-14 20-21 20-25

21-22 22-23 23-24 24-25

exact/norm bonds :

11-15 15-16 17-18 18-19

exact bonds :

4-7 7-8 8-14 16-17 18-26 19-22 28-29

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 9-10 9-14 10-11 11-12 12-13 13-14 20-21 20-25

21-22 22-23 23-24 24-25

isolated ring systems : containing 1 : 9 : 20 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:Atom 10:Atom

11:Atom 12:Atom 13:Atom 14:Atom 15:CLASS 16:CLASS 17:CLASS 18:CLASS

19:CLASS 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:CLASS 28:CLASS

29:CLASS 30:CLASS

L5 STRUCTURE UPLOADED

=> d 15

L5 HAS NO ANSWERS

L5 STR

Structure attributes must be viewed using STN Express query preparation.

SAMPLE SEARCH INITIATED 08:44:05 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED -9 TO ITERATE

100.0% PROCESSED

9 ITERATIONS

0 ANSWERS

10626155.trn Page 33

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 9 TO 360 PROJECTED ANSWERS: 0 TO 0

L6 0 SEA SSS SAM L5

=> s 15 sss full

=> FIL HCAPLUS

FULL SEARCH INITIATED 08:44:12 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 327 TO ITERATE

100.0% PROCESSED 327 ITERATIONS

SEARCH TIME: 00.00.01

L7 12 SEA SSS FUL L5

COST IN U.S. DOLLARS SINCE FILE TOTAL

FULL ESTIMATED COST ENTRY SESSION 161.33 367.13

12 ANSWERS

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE TOTAL ENTRY SESSION

CA SUBSCRIBER PRICE 0.00 -2.92

FILE 'HCAPLUS' ENTERED AT 08:44:18 ON 30 AUG 2005 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 30 Aug 2005 VOL 143 ISS 10 FILE LAST UPDATED: 29 Aug 2005 (20050829/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 17 L8

=> d 18 ibib abs hitstr tot

L8 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2005:78301 HCAPLUS

DOCUMENT NUMBER: 142:176433

10626155.trn

Page 34

08/30/2005

10626155.trn

TITLE:

A preparation of acetylenic compounds, useful in the treatment of inflammatory disorders

INVENTOR (S):

Beers, Scott; Malloy, Elizabeth A.; Wachter, Michael

ΙI

PATENT ASSIGNEE (S

SOURCE:

U.S. Pat. Appl. Publ., 19 pp.

CODEN: USXXCO

DOCUMENT TYPE:

Patent

USA****

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005020838	A1	20050127	US 2003-626155	20030724
PRIORITY APPLN. INFO.:			US 2003-626155	20030724
OTHER SOURCE(S):	MARPAT	142:176433		
GI				

$$R^{1}$$
 A
 M
 H
 O
 B
 C
 C
 X
 E
 $(R^{4})_{1?5}$
 I

$$C1$$
 $C\equiv C$ Me NH_2 Me NH_2

AB The invention relates to a preparation of acetylenic compds. of formula I [wherein: A is cycloalkyldiyl, cyclic heteroalkyldiyl, or (hetero)aryldiyl; B is (hetero)aryldiyl; E is (hetero)aryldiyl; M and X are independently (CH2)0-4; R1 is cycloalkyl, cyclic heteroalkyl, or (hetero)aryl, etc.; R2 is H, alkyl, alkoxy, CHO, CO2H, or NH2, etc.; R3 and R4 are independently H, alkyl, CHO, cycloalkyl, or aryl, etc.], useful in the treatment of inflammatory disorders. For instance, acetylene derivative II (oxidase inhibition: IC50 = $0.7 \mu M$) was prepared via reductive amination of ketone III by 1,4-bis(aminomethyl)benzene.

ΙT 651330-36-8P 651330-37-9P 651330-38-0P 651330-39-1P 651330-68-6P 773847-69-1P 776293-45-9P 792905-81-8P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

10626155.trn

Page 35

(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of acetylenic compound useful in the treatment of inflammatory disorders)

RN 651330-36-8 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[4-[(4-chlorophenyl)ethynyl]-2-methylphenoxy]-1-methylethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{O-CH}_2\text{-CH-NH-CH}_2 \\ \end{array}$$

RN 651330-37-9 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[4-[(4-chlorophenyl)ethynyl]-2-methylphenoxy]-1-methylethyl]-, dihydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{C1} \\ \text{C2} \\ \text{C2} \\ \text{C3} \\ \text{C4} \\ \text{C1} \\ \text{C2} \\ \text{C4} \\ \text{C2} \\ \text{C2} \\ \text{C4} \\ \text{C2} \\ \text{C2} \\ \text{C3} \\ \text{C4} \\ \text{C5} \\ \text{C6} \\ \text{C7} \\ \text{C6} \\ \text{C7} \\ \text{C7} \\ \text{C7} \\ \text{C7} \\ \text{C8} \\$$

●2 HCl

RN 651330-38-0 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[2-chloro-4-(phenylethynyl)phenoxy]-1-methylethyl]- (9CI) (CA INDEX NAME)

RN 651330-39-1 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[1-[[4-[(4-chlorophenyl)ethynyl]-2-methylphenoxy]methyl]propyl]- (9CI) (CA INDEX NAME)

C1
$$CH_2-NH_2$$
 CH_2-NH_2 CH_2-NH_2

RN 651330-68-6 HCAPLUS

10626155.trn

Page 36

CN 1,4-Benzenedimethanamine, N-[2-[4-[(4-chlorophenyl)ethynyl]-2-methylphenoxy]ethyl]- (9CI) (CA INDEX NAME)

$$H_2N-CH_2$$
 $CH_2-NH-CH_2-CH_2-O$
 $CH_2-NH-CH_2-CH_2-O$

RN 773847-69-1 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[2-chloro-4-[(4-fluorophenyl)ethynyl]phenoxy]-1-methylethyl]- (9CI) (CA INDEX NAME)

RN 776293-45-9 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[2-chloro-4-[(4-chlorophenyl)ethynyl]phenoxy]-1-methylethyl]- (9CI) (CA INDEX NAME)

C1
$$Me$$
 CH_2-NH_2 CH_2-NH_2

RN 792905-81-8 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[2-chloro-4-[(4-methylphenyl)ethynyl]phenoxy]-1-methylethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{C1} & \text{Me} \\ \text{O-CH}_2\text{-CH-NH-CH}_2 \\ \end{array}$$

L8 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:80636 HCAPLUS

DOCUMENT NUMBER: 140:145889

TITLE: Preparation of acetylenic-aryl-methylamines useful in

treating inflammatory disorders

INVENTOR(S): Beers, Scott; Malloy, Elizabeth A.; Wachter, Michael

Р.

PATENT ASSIGNEE(S): Janssen Pharmaceutica N.V., Belg.

SOURCE: PCT Int. Appl., 61 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

10626155.trn Page 37 08:44

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE -------------------WO 2004009531 **A1** 20040129 WO 2003-US23140 20030724 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG PRIORITY APPLN. INFO.: US 2002-398138P P. 20020724 OTHER SOURCE(S): MARPAT 140:145889 GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [A = cycloalkyldiyl, cyclic heteroalkyldiyl, etc.; B, E = (hetero)aryldiyl; R1 = cycloalkyl, cyclic heteroalkyl, heteroaryl, etc.; R2 = H, alkanyl, alkoxy, acyl, etc.; R3-4 = H, alkanyl, carboxy, cycloalkyl, etc.] are prepared For instance, 4-iodo-2-methylphenol is alkylated with chloroacetone (acetone, K2CO3, NaI, reflux, 18 h), the product coupled to 4-chlorophenylacetylene (Pd(II), Et3N) and used to alkylate p-xylylene diamine (CH2Cl2, HOAc, NaBH(OAc)3) to give II. In an NADPH oxidase assay for inhibition of superoxide-mediated reduction of cytochrome C in human neutrophils incubated with phorbol myristate acetate, 26 compds. I had IC50 values of 0.7-11.13 μM; II had IC50 = 0.7 μM. I are useful in treating or ameliorating reactive oxygen species-mediated inflammatory disorders.

IT 651330-36-8P 651330-37-9P 651330-38-0P 651330-39-1P 651330-40-4P 651330-41-5P 651330-42-6P 651330-43-7P 651330-68-6P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of acetylenic-aryl-methylamines as NAD oxidase hydride donor inhibitors useful in treating reactive oxygen species-mediated inflammatory disorders)

RN 651330-36-8 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[4-[(4-chlorophenyl)ethynyl]-2-methylphenoxy]-1-methylethyl]- (9CI) (CA INDEX NAME)

RN 651330-37-9 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[4-[(4-chlorophenyl)ethynyl]-2-methylphenoxy]-1-methylethyl]-, dihydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{C1} \\ \text{C2} \\ \text{C3} \\ \text{C4} \\ \text{C1} \\ \text{C2} \\ \text{C4} \\ \text{C1} \\ \text{C2} \\ \text{C2} \\ \text{C2} \\ \text{C2} \\ \text{C3} \\ \text{C4} \\ \text{C5} \\ \text{C6} \\ \text{C7} \\ \text{C6} \\ \text{C7} \\ \text{C7} \\ \text{C7} \\ \text{C8} \\$$

●2 HCl

RN 651330-38-0 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[2-chloro-4-(phenylethynyl)phenoxy]-1-methylethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{CH}_2\text{N-CH}_2 \\ \text{CH}_2\text{-NH-CH-CH}_2\text{-O} \\ \text{Cl} \end{array}$$

RN 651330-39-1 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[1-[[4-[(4-chlorophenyl)ethynyl]-2-methylphenoxy]methyl]propyl]- (9CI) (CA INDEX NAME)

RN 651330-40-4 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[1-[[4-[(4-chlorophenyl)ethynyl]-2-methylphenoxy]methyl]propyl]-, dihydrochloride (9CI) (CA INDEX NAME)

C1
$$CH_2-NH_2$$
 CH_2-NH_2 CH_2-NH_2

●2 HCl

RN 651330-41-5 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[2-chloro-4-[(4-methylphenyl)ethynyl]phenoxy]-1-methylethyl]-, dihydrochloride (9CI) (CAINDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{O-CH}_2\text{-CH-NH-CH}_2 \\ \end{array}$$

●2 HCl

RN 651330-42-6 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[2-chloro-4-[(4-chlorophenyl)ethynyl]phenoxy]-1-methylethyl]-, dihydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{C1} & \text{Me} \\ \text{O-CH}_2\text{-CH-NH-CH}_2 \end{array}$$

●2 HC1

RN 651330-43-7 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[2-chloro-4-[(4-fluorophenyl)ethynyl]phenoxy]-1-methylethyl]-, dihydrochloride (9CI) (CA INDEX NAME)

●2 HCl

RN 651330-68-6 HCAPLUS

CN 1,4-Benzenedimethanamine, N-[2-[4-[(4-chlorophenyl)ethynyl]-2-methylphenoxy]ethyl]- (9CI) (CA INDEX NAME)

$$H_2N-CH_2$$
 $CH_2-NH-CH_2-CH_2-O$
 C

REFERENCE COUNT:

THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> log y COST IN U.S. DOLLARS	SINCE FILE	TOTAL
COST IN C.S. DOLLARS	ENTRY	SESSION
FULL ESTIMATED COST	12.33	379.46
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-1.46	-4.38

STN INTERNATIONAL LOGOFF AT 08:44:54 ON 30 AUG 2005

5